

Nitrofurantoin  
67-20-9 | DTXSID7020972

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

## Model Results

**Predicted value:** 2.57e-11 cm<sup>3</sup>/molecule\*sec

**Global applicability domain:** Outside

**Local applicability domain index:** 1.33e-01

**Confidence level:** 6.14e-01

## Nearest Neighbors from the Training Set

Image not found

2-Methyl-p-benzoquinone

**Measured:** 2.35e-11

**Predicted:** 2.15e-11

Image not found

2,5-Furandione

**Measured:** 1.45e-12

**Predicted:** 2.17e-12